SEARCH REQUEST FORM

Scientific and Technical Inf rmation Center

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Requester's Full Name:	erst.	Examiner #: $\frac{599}{2}$	Date: 4/29/63
	Jumber 30 0 453	Serial Number: 6	9/895812
Mail Box and Bldg/Room Location	Resu	ilts Format Preferred (circle): 4	APER DISK E-MAIL
3D(9)	1007		•
If more than one search is subm	rtted, please prioritiz	e searches in order of need]. *********
Please provide a detailed statement of the			
Include the elected species or structures, k utility of the invention. Define any terms	eywords, synonyms, acron	yms, and registry numbers, and con	bine with the concept or
known. Please attach a copy of the cover s			itations, authors, etc., if
Title of Invention:		Square ~	
Inventors (please provide full names): _		<i>y</i> ,	<u> </u>
			*
Earliest Priority Filing Date:			
For Sequence Searches Only Please include	le all pertinent information (j	— parent, child, divisional, or issued pate	nt numbers) along with the
appropriate serial number.			
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A CONTRACTOR OF THE PROPERTY O		1E07 – 703-308-4498 a.delavai@uspto.gov	
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STAFF USE ONLY	Type of Search	Vendors and cost where	e applicable
Searcher:	NA Sequence (#)	STN V	
Searcher Phone #:	AA Sequence (#)	Dialog	·
Searcher Location:	Structure (#)	Questel/Orbit	
Date Searcher Picked Up: 4/26/53	Bibliographic	Dr.Link	<u>·</u>
Date Completed: 4126 (73	Litigation	Lexis/Nexis	<u> </u>
Searcher Prep & Review Time:	Fulltext	Sequence Systems	<u> </u>
Clerical Prep Time: 10	Patent Family	WWW/Internet	

PTO-1590 (8-01)

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BioTech-Chem Library Search Results Feedback Form (Optional)



The search results generated for your recent request are attached. If you have any questions or comments (compliments or complaints) about the scope or the results of the search, please contact *the BioTech-Chem searcher* who conducted the search *or contact*:

Mary Hale, Supervisor, 308-4258 CM-1 Room 1E01

Voluntary Results Feedback Form
> I am an examiner in Workgroup: (Example: 1610)
> Relevant prior art found, search results used as follows:
102 rejection
103 rejection
Cited as being of interest.
Helped examiner better understand the invention.
Helped examiner better understand the state of the art in their technology.
Types of relevant prior art found
Foreign Patent(s)
Non-Patent Literature (journal articles, conference proceedings, new product announcements etc.)
> Relevant prior art not found:
Results verified the lack of relevant prior art (helped determine patentability).
Search results were not useful in determining patentability or understanding the invention.
Other Comments:

Drop off completed forms at the Circulation Desk CM-1, or send to Mary Hale, CM1-1E01 or e-mail mary hale@uspto.gov.

=> fil reg FILE 'REGISTRY' ENTERED AT 12:18:00 ON 29 APR 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 APR 2003 HIGHEST RN 506405-59-0 DICTIONARY FILE UPDATES: 27 APR 2003 HIGHEST RN 506405-59-0

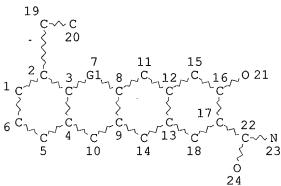
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d sta que 16 L1 STR



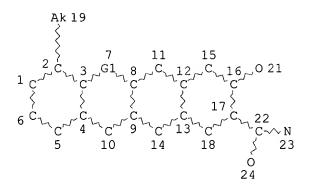
VAR G1=C/O/N/S NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L3 166 SEA FILE=REGISTRY SSS FUL L1 L4 STR

Jan Delaval
Reference Librarian
Biotechnology & Chemical Library
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jan.delaval@uspto.gov



VAR G1=C/O/N/S
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT IS UNS AT 19
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 2

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

L6 91 SEA FILE=REGISTRY SUB=L3 SSS FUL L4

100.0% PROCESSED 166 ITERATIONS 91 ANSWERS

SEARCH TIME: 00.00.01

=> d his 16-

(FILE 'REGISTRY' ENTERED AT 12:12:19 ON 29 APR 2003)

L6 91 S L4 FUL SUB=L3

SAV L6 GERSTL895A/A TEMP

L7 75 S L3 NOT L6

FILE 'HCAPLUS' ENTERED AT 12:15:00 ON 29 APR 2003

L8 9 S L6

L9 6 S L7

L10 6 S L8 AND L9

L11 9 S L8-L10

L12 9 S L11 AND (NELSON ? OR FRECHETTE ? OR VISKI ? OR ISMAIL ? OR BO

FILE 'HCAPLUS' ENTERED AT 12:17:19 ON 29 APR 2003

FILE 'USPATFULL, USPAT2' ENTERED AT 12:17:23 ON 29 APR 2003

L13 3 S L6

L14 2 S L7

L15 3 S L13, L14

FILE 'HCAPLUS, USPATFULL' ENTERED AT 12:17:39 ON 29 APR 2003 L16 12 DUP REM L12 L15 (O DUPLICATES REMOVED)

FILE 'REGISTRY' ENTERED AT 12:18:00 ON 29 APR 2003

=> fil uspatall

FILE 'USPATFULL' ENTERED AT 12:18:15 ON 29 APR 2003

CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

FILE 'USPAT2' ENTERED AT 12:18:15 ON 29 APR 2003 CA INDEXING COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

```
=> d l15 bib abs hitrn fhitstr tot
    ANSWER 1 OF 3 USPATFULL
L15
ΑN
       2003:79098 USPATFULL
ΤI
       7-substituted tetracycline compounds
ΙN
       Nelson, Mark L., Wellesley, MA, UNITED STATES
       Frechette, Roger, Reading, MA, UNITED STATES
       Viski, Peter, Brookline, MA, UNITED STATES
       Ismail, Mohamed, Bedrford, MA, UNITED STATES
       Bowser, Todd, Charlton, MA, UNITED STATES
       Bhatia, Beena, Arlington, MA, UNITED STATES
       Messersmith, David, Somerville, MA, UNITED STATES
       McIntyre, Laura, Arlington, MA, UNITED STATES
       Koza, Darrell, Westerly, RI, UNITED STATES
       Rennie, Glen, Weymouth, MA, UNITED STATES
       Sheahan, Paul, Hopkinton, MA, UNITED STATES
       Hawkins, Paul, Cambridge, MA, UNITED STATES
       Verma, Atul, Arlington, MA, UNITED STATES
       Warchol, Tadeusz, Acton, MA, UNITED STATES
       Bandarage, Upul, Newton, MA, UNITED STATES
PΙ
       US 2003055025
                          A1
                              20030320
ΑI
       US 2001-895812
                          A1
                               20010629 (9)
PRAI
       US 2001-275576P
                           20010313 (60)
       US 2000-216760P
                           20000707 (60)
DT
       Utility
FS
       APPLICATION
       Elizabeth A. Hanley, Esq., Lahive & Cockfield, LLP, 28 State Street,
LREP
       Boston, MA, 02109
       Number of Claims: 88
CLMN
ECL
       Exemplary Claim: 1
DRWN
       No Drawings
LN.CNT 2462
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB
       The present invention pertains, at least in part, to novel 7-substituted
       tetracycline compounds. These tetracycline compounds can be used to
       treat numerous tetracycline compound-responsive states, such as
       bacterial infections and neoplasms, as well as other known applications
       for minocycline and tetracycline compounds in general, such as blocking
       tetracycline efflux and modulation of gene expression.
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT
     389624-36-6P
        (prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as
        antibacterial agents)
ΙT
     389623-84-1P 389623-86-3P 389623-89-6P
      389623-90-9P 389623-91-0P 389623-98-7P
      389623-99-8P 389624-00-4P 389624-01-5P
      389624-02-6P 389624-06-0P 389624-08-2P
      389624-09-3P 389624-10-6P 389624-11-7P
      389624-14-0P 389624-15-1P 389624-16-2P
      389624-17-3P 389624-18-4P 389624-19-5P
      389624-20-8P 389624-25-3P 389624-26-4P
      389624-27-5P 389624-30-0P 389624-31-1P
      389624-32-2P 389624-33-3P 389624-35-5P
      389624-37-7P 389624-38-8P 389624-39-9P
      389624-40-2P 389624-41-3P 389624-42-4P
      389624-43-5P 389624-44-6P 389624-46-8P
      389624-47-9P 389624-48-0P 389624-49-1P'
```

389624-50-4P 389624-51-5P 389624-52-6P 389624-53-7P 389624-56-0P 389624-60-6P

```
389624-61-7P 389624-62-8P 389624-63-9P
389624-64-0P 389624-65-1P 389624-66-2P
389624-67-3P 389624-68-4P 389624-70-8P
389624-71-9P 389624-72-0P 389624-73-1P
389624-74-2P 389624-75-3P 389624-76-4P
389624-77-5P 389624-78-6P 389624-79-7P
389624-80-0P 389624-83-3P 389624-84-4P
389624-85-5P 389624-86-6P 389624-87-7P
389624-88-8P 389624-89-9P 389624-95-7P
389624-96-8P
```

(prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

TΤ 389624-36-6P

L15

CLMN

(prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

RN 389624-36-6 USPATFULL

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[(3-methoxyphenyl)ethynyl]-1,11-dioxo-, (4S, 4aS, 5aR, 12aS) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

```
ANSWER 2 OF 3 USPATFULL
AN
       2002:337989 USPATFULL
TΙ
       7, 9-substituted tetracycline compounds
IN
       Nelson, Mark L., Wellesley, MA, UNITED STATES
       Frechette, Roger, Reading, MA, UNITED STATES
       Viski, Peter, Brookline, MA, UNITED STATES
       Ismail, Mohamed, Bedford, MA, UNITED STATES
       Bowser, Todd, Charlton, MA, UNITED STATES
       McIntyre, Laura, Arlington, MA, UNITED STATES
       Bhatia, Beena, Arlington, MA, UNITED STATES
       Hawkins, Paul, Cambridge, MA, UNITED STATES
       Reddy, Laxma, Lexington, MA, UNITED STATES
       Stapleton, Karen, Weymouth, MA, UNITED STATES
       Warchol, Tad, Acton, MA, UNITED STATES
       Sheahan, Paul, Hopkinton, MA, UNITED STATES
PΙ
       US 2002193354
                          A1
                                20021219
ΑI
       US 2001-895797
                                20010629 (9)
                          A1
PRAI
       US 2001-275620P
                           20010313 (60)
DT
       Utility
FS
       APPLICATION
LREP
       Elizabeth A. Hanley, Esq., Lahive & Cockfield, LLP, 28 State Street,
       Boston, MA, 02109
```

Number of Claims: 61

```
ECL Exemplary Claim: 1
```

DRWN No Drawings

LN.CNT 1511

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

The present invention pertains to novel 7,9-substituted tetracycline compounds. These tetracycline compounds can be used to treat numerous tetracycline compound-responsive states, such as bacterial infections and neoplasms, as well as other known applications for minocycline and tetracycline compounds in general, such as blocking tetracycline efflux and modulation of gene expression.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 459810-04-9P

(prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

IT 459809-43-9P 459809-46-2P 459809-47-3P

459809-48-4P 459809-51-9P 459809-54-2P

459809-56-4P 459809-58-6P 459809-61-1P

459809-63-3P 459809-65-5P 459809-67-7P

459809-70-2P 459809-72-4P 459809-81-5P

459809-86-0P 459809-92-8P 459809-94-0P

459809-99-5P 459810-03-8P 459810-05-0P

459810-06-1P 459810-09-4P

(prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

IT 263761-05-3P, 7-Ethynylsancycline 389624-14-0P,

7-Ethylsancycline 459810-10-7P

(prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use, as antibacterial agents)

IT 459810-04-9P

(prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

RN 459810-04-9 USPATFULL

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-ethyl-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-9-iodo-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

```
L15 ANSWER 3 OF 3 USPATFULL
```

AN 2002:206638 USPATFULL

TI 7,8 and 9-substituted tetracycline compounds

IN Nelson, Mark L., Wellesley, MA, UNITED STATES

Koza, Darrell, Westerly, RI, UNITED STATES

PI US 2002111335 A1 20020815

AI US 2001-894805 A1 20010629 (9) PRAI WO 2000-US21366 20000804

US 2000-216656P 20000707 (60)

DT Utility

FS APPLICATION

LREP LAHIVE & COCKFIELD, 28 STATE STREET, BOSTON, MA, 02109

CLMN Number of Claims: 26 ECT. Exemplary Claim: 1

DRWN No Drawings

LN.CNT 1042

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

7, 8 and 9-substituted tetracycline compounds, methods of treating AR tetracycline responsive states, and pharmaceutical compositions containing the 7, 8 and 9-substituted tetracycline compounds are described.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

263761-03-1P 389570-50-7P 389570-53-0P

(prepn. of 7,8 and 9-substituted tetracycline derivs. as antibacterial agents)

ΙT 263761-03-1P

> (prepn. of 7,8 and 9-substituted tetracycline derivs. as antibacterial agents)

263761-03-1 USPATFULL RN

2-Naphthacenecarboxamide, 4-(dimethylamino)-7-ethenyl-1,4,4a,5,5a,6,11,12a-CN octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

=> fil hcaplus

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FILE COVERS 1907 - 29 Apr 2003 VOL 138 ISS 18 FILE LAST UPDATED: 28 Apr 2003 (20030428/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

```
ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2003 ACS
L12
     2003:57866 HCAPLUS
ΑN
     138:117673
DN
ΤI
     Tetracycline compounds having target therapeutic activities
     Levy, Stuart B.; Draper, Michael; Nelson, Mark L.; Jones, Graham
IN
     Paratek Pharmaceuticals, Inc., USA
PΑ
     PCT Int. Appl., 158 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
ICI
    A61
CC
     1-12 (Pharmacology)
     Section cross-reference(s): 26
FAN.CNT 1
                      KIND DATE
                                           APPLICATION NO.
                                                             DATE
     PATENT NO.
                      ____
                            -----
     WO 2003005971
                            20030123
                                           WO 2002-US22451 20020715
                       Α2
PΙ
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
             UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
             CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
             PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,
             NE, SN, TD, TG
                            20010713
PRAI US 2001-305546P
     MARPAT 138:117673
OS
     Methods and compds. for treating a variety of diseases with tetracycline
AB
     compds. having a target therapeutic activity are described, as is compd.
ST
     tetracycline compd prepn therapeutic
ΙT
     Brain, disease
     Prion diseases
        (Creutzfeldt-Jakob; tetracycline compds. with target therapeutic
        activities)
ΙT
     Nervous system
        (GABAergic, GABAergic therapy; tetracycline compds. with target
        therapeutic activities, and use with other agents)
IT
     Brain, disease
        (Gilles de la Tourette syndrome; tetracycline compds. with target
        therapeutic activities)
ΙT
     Nervous system
        (Huntington's chorea; tetracycline compds. with target therapeutic
        activities)
     Wernicke-Korsakoff syndrome
ΙT
        (Korsakoff's psychosis; tetracycline compds. with target therapeutic
        activities)
TT
     Amnesia
        (Korsakoff's; tetracycline compds. with target therapeutic activities)
TT
     Glutamate antagonists
        (NMDA antagonists; tetracycline compds. with target therapeutic
        activities, and use with other agents)
     Inflammation
IT
     Respiratory distress syndrome
        (acute; tetracycline compds. with target therapeutic activities)
ΙT
     Respiratory distress syndrome
        (adult; tetracycline compds. with target therapeutic activities)
ΙT
     Nervous system
        (amyotrophic lateral sclerosis; tetracycline compds. with target
        therapeutic activities)
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```
ΙT
    Artery, disease
        (aneurism; tetracycline compds. with target therapeutic activities)
IT
    Antiarteriosclerotics
        (antiatherosclerotics; tetracycline compds. with target therapeutic
        activities)
    Artery, disease
ΙT
        (aorta, aneurism; tetracycline compds. with target therapeutic
        activities)
    Mental disorder
ΙT
        (attention deficit disorder; tetracycline compds. with target
        therapeutic activities)
ΙT
    Glycosylation
        (biol., protein; tetracycline compds. with target therapeutic
        activities)
TΤ
    Bone, disease
        (bone mass disorder; tetracycline compds. with target therapeutic
        activities)
    Bronchi
TΤ
        (bronchiectasis; tetracycline compds. with target therapeutic
        activities)
ΙT
    Bronchi, disease
        (bronchitis; tetracycline compds. with target therapeutic activities)
ΙT
     Ion channel blockers
        (calcium; tetracycline compds. with target therapeutic activities, and
        use with other agents)
    Musculoskeletal diseases
ΙT
        (cartilage, degrdn.; tetracycline compds. with target therapeutic
        activities)
IT
    Lung, disease
        (chronic obstructive; tetracycline compds. with target therapeutic
        activities)
ΙT
    Inflammation
    Lung, disease
        (chronic; tetracycline compds. with target therapeutic activities)
ΙT
    Animal cell
        (compds. increasing energy available to cells; tetracycline compds.
        with target therapeutic activities, and use with other agents)
ΙT
    Eye, disease
        (cornea, ulcer; tetracycline compds. with target therapeutic
        activities)
ΙT
    Antiulcer agents
        (corneal ulceration; tetracycline compds. with target therapeutic
        activities)
IT
    Bone, disease
        (degrdn.; tetracycline compds. with target therapeutic activities)
ΙT
    Mental disorder
        (dementia, Alzheimer's disease-related; tetracycline compds. with
        target therapeutic activities)
IT
    Mental disorder
        (depression, major; tetracycline compds. with target therapeutic
        activities)
TΤ
    Mental disorder
        (depression, neurotic; tetracycline compds. with target therapeutic
       activities)
IΤ
    Mental disorder
        (depression; tetracycline compds. with target therapeutic activities)
ΙT
    Disease, animal
        (diabetic complications; tetracycline compds. with target therapeutic
        activities)
    Ulcer
TΥ
        (diabetic; tetracycline compds. with target therapeutic activities)
IT
    Cartilage
```

(disease, degrdn.; tetracycline compds. with target therapeutic

```
activities)
ΙT
    Nervous system
        (disease; tetracycline compds. with target therapeutic activities)
IT
     Learning
     Sleep
        (disorder; tetracycline compds. with target therapeutic activities)
ΙT
     Eye, disease
        (dry; tetracycline compds. with target therapeutic activities)
ΙT
        (gastrointestinal; tetracycline compds. with target therapeutic
        activities)
ΙT
     Proteins
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (glycosylation; tetracycline compds. with target therapeutic
        activities)
IT
     Disease, animal
        (inflammation process-assocd. state; tetracycline compds. with target
        therapeutic activities)
IT
     Lung, disease
        (injury, acute; tetracycline compds. with target therapeutic
        activities)
IT
     Brain, disease
     Nerve, disease
        (injury; tetracycline compds. with target therapeutic activities)
IT
     Diabetes mellitus
        (insulin-dependent; tetracycline compds. with target therapeutic
        activities)
IT
    Mental disorder
        (mania; tetracycline compds. with target therapeutic activities)
ΙT
        (manic bipolar disorder; tetracycline compds. with target therapeutic
        activities)
ΙT
     Neoplasm
        (metastasis; tetracycline compds. with target therapeutic activities)
IT
        (migraine; tetracycline compds. with target therapeutic activities)
ΙT
     Nerve, disease
        (motor; tetracycline compds. with target therapeutic activities)
ΙT
        (neuron, neuronal membrane stabilizers; tetracycline compds. with
        target therapeutic activities, and use with other agents)
ΙT
    Membrane, biological
        (neuronal membrane stabilizers; tetracycline compds. with target
        therapeutic activities, and use with other agents)
ΙT
     Cytoprotective agents
        (neuroprotectants; tetracycline compds. with target therapeutic
        activities, and use with other agents)
ΙT
    Mental disorder
        (obsession-compulsion; tetracycline compds. with target therapeutic
        activities)
IT
     Bone, neoplasm
        (osteosarcoma; tetracycline compds. with target therapeutic activities)
ΙT
        (panic disorder; tetracycline compds. with target therapeutic
        activities)
IT
     Periodontium
        (periodontitis; tetracycline compds. with target therapeutic
        activities)
ΙT
    Mental disorder
        (phobia; tetracycline compds. with target therapeutic activities)
     Fatty acids, biological studies
TΤ
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
```

(polyunsatd., n-3; tetracycline compds. with target therapeutic activities, and use with other agents) ΙT Proteins RL: BSU (Biological study, unclassified); BIOL (Biological study) (protein buildup removal agents; tetracycline compds. with target therapeutic activities, and use with other agents) IT(pseudobulbar; tetracycline compds. with target therapeutic activities) ITTranscription, genetic (regulators; tetracycline compds. with target therapeutic activities, and use with other agents) ITArtery, disease (restenosis; tetracycline compds. with target therapeutic activities) ΙT (schizoaffective disorder; tetracycline compds. with target therapeutic activities) IT Mental disorder (senile psychosis; tetracycline compds. with target therapeutic activities) ΙT Respiratory tract (sinusitis; tetracycline compds. with target therapeutic activities) ΙT Ion channel blockers (sodium; tetracycline compds. with target therapeutic activities, and use with other agents) ITBrain, disease (stroke; tetracycline compds. with target therapeutic activities) ΙT Aging, animal Alzheimer's disease Amnesia Aneurysm Angiogenesis Angiogenesis inhibitors Anti-Alzheimer's agents Anti-inflammatory agents Anti-ischemic agents Antiarteriosclerotics Antiarthritics Antiasthmatics Antibacterial agents Anticonvulsants Antidepressants Antidiabetic agents Antihypertensives Antimalarials Antimigraine agents Antipsychotics Antirheumatic agents Antitumor agents Antiviral agents Anxiety Anxiolytics Arteriosclerosis Asthma Atherosclerosis Autoimmune disease Carcinoma Cardiovascular agents Cognition enhancers Cystic fibrosis Diabetes mellitus Drug delivery systems Emphysema

Epilepsy

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Escherichia coli
     Eye, disease
     Fungicides
     Hepatitis
     Human
     Hypertension
     Inflammation
     Ischemia
     Lung, disease
     Macrophage
     Malaria
     Mental disorder
     Multiple sclerosis
     Neoplasm
     Nervous system agents
     Osteoarthritis
     Osteomyelitis
     Osteoporosis
     Parasiticides
     Psychotropics
     Rheumatoid arthritis
     Sarcoma
     Schizophrenia
     Skin, disease
     Staphylococcus aureus
     Wound healing promoters
        (tetracycline compds. with target therapeutic activities)
ΙT
     Tetracyclines
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (tetracycline compds. with target therapeutic activities)
     Anti-infective agents
IT
     Antioxidants
     Chemotherapy
     Ginkgo biloba
     Opioid antagonists
     Radiotherapy
        (tetracycline compds. with target therapeutic activities, and use with
        other agents)
IT
     Glucocorticoids
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (tetracycline compds. with target therapeutic activities, and use with
        other agents)
IT
        (tissue; tetracycline compds. with target therapeutic activities)
IT
     Brain, disease
     Spinal cord
        (trauma; tetracycline compds. with target therapeutic activities)
IT
     Intestine, disease
        (ulcerative colitis; tetracycline compds. with target therapeutic
        activities)
IT
     Blood vessel, disease
        (vascular stroke; tetracycline compds. with target therapeutic
        activities)
IT
     Tumor necrosis factors
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (.alpha., antagonists; tetracycline compds. with target therapeutic
        activities, and use with other agents)
IT
     141907-41-7, Matrix metalloproteinase
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (MMP-4 and MMP5, inflammatory process-assocd. state assocd. with;
        tetracycline compds. with target therapeutic activities)
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ΙT
     10102-43-9, Nitric oxide, biological studies
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (NO-assocd. state; tetracycline compds. with target therapeutic
        activities)
ΙT
     56-86-0, L-Glutamic acid, biological studies
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (anti-glutamate therapy; tetracycline compds. with target therapeutic
        activities, and use with other agents)
IT
     9001-12-1, Matrix metalloproteinase 1
                                              9004-06-2, Matrix
     metalloproteinase 12
                             79955-99-0, Matrix metalloproteinase 3
     140610-48-6, Matrix metalloproteinase 10
                                                 141256-52-2, Matrix
     metalloproteinase 7
                           145267-01-2, Matrix metalloproteinase 11
     146480-35-5, Matrix metalloproteinase 2
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     172308-17-7, Matrix metalloproteinase 15
                                                  175449-82-8, Matrix
     metalloproteinase 13
                             182970-56-5, Matrix metalloproteinase 16
     185766-51-2, Matrix metalloproteinase 20
                                                 188364-80-9, Matrix
     metalloproteinase 19
                             203810-08-6, Matrix metalloproteinase 17
     252351-86-3, Matrix metalloproteinase 6
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (inflammatory process-assocd. state assocd. with; tetracycline compds.
        with target therapeutic activities)
ΙT
     9001-08-5, Cholinesterase
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (inhibitors; tetracycline compds. with target therapeutic activities,
        and use with other agents)
                    488820-35-5P
                                    488820-36-6P
                                                    488820-38-8P
TT
     389624-49-1P
     488820-39-9P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (tetracycline compds. with target therapeutic activities)
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               60-54-8D, Tetracycline, derivs.
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     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (tetracycline compds. with target therapeutic activities)
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     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (tetracycline compds. with target therapeutic activities)
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         (tetracycline compds. with target therapeutic activities)
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        (tetracycline compds. with target therapeutic activities)
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        (tetracycline compds. with target therapeutic activities)
                        100-39-0, Benzyl bromide
                                                  103-55-9
IT
    74-99-7, Propyne
                                                              111-30-8,
                      122-78-1, Phenylacetaldehyde
                                                     622-77-5, Benzylcyanamide
    Glutaraldehyde
                           871-84-1, 1,7-Octadiyne
    808-26-4, Sancycline
                                                      5371-49-3
                                                                  13614-98-7,
    Minocycline hydrochloride 25154-38-5, Piperazineethanol
                                                                  25267-27-0,
                  50696-61-2, Cyclohexenylacetylene
                                                      55552-70-0, 3-Furanyl
    Iodobutane
                    107099-99-0, 2,5-Dimethoxyphenyl boronic acid
    boronic acid
    128796-39-4, 4-Trifluoromethylphenyl boronic acid
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    2,4-Difluorophenyl boronic acid
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     (Reactant or reagent)
        (tetracycline compds. with target therapeutic activities)
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ΙT
    50-81-7, Vitamin C, biological studies
                                             53-03-2, Prednisone
    Retinoic acid
                     303-98-0, Coenzyme Q10
                                              987-78-0, CDP-choline
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    1134-47-0, Baclofen
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    2763-96-4, Muscimol
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    Gabapentin
    128298-28-2, Remacemide
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     (Biological study); USES (Uses)
        (tetracycline compds. with target therapeutic activities, and use with
        other agents)
IT
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     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (tetracycline compds. with target therapeutic activities)
RN
     389624-49-1 HCAPLUS
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CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[2-(4-methylphenyl)ethyl]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2003 ACS
L12
ΑN
     2002:832571 HCAPLUS
DN
     137:333118
     Substituted tetracycline compounds for the treatment of malaria
TΙ
     Draper, Michael; Nelson, Mark L.; Frechette, Roger
IN
PA
     Paratek Pharmaceuticals, Inc., USA
SO
     PCT Int. Appl., 89 pp.
     CODEN: PIXXD2
DΤ
     Patent
LA
     English
IC
     ICM A61K
     1-5 (Pharmacology)
     Section cross-reference(s): 25, 63
FAN.CNT 1
                                           APPLICATION NO.
     PATENT NO.
                      KIND
                            DATE
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                                                            20020424
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             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
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PRAI US 2001-286193P
                            20010424
OS
     MARPAT 137:333118
AB
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AB The invention provides a method for treating or preventing malaria in a subject. The method includes administering to the subject an effective amt. of a substituted tetracycline compd., such that malaria is treated or prevented. In one aspect, the invention provides pharmaceutical compns. which include an effective amt. of a tetracycline compd. to treat malaria in a subject and a pharmaceutically acceptable carrier. The substituted tetracycline compds. of the invention can be used in combination with one or more antimalarial compds. or can be used to treat or prevent malaria

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which is resistant to one or more other antimalarial compds.
    prepn. is described.
ST
    tetracycline deriv prepn antimalarial; malaria treatment tetracycline
    deriv
ΙT
    Antimalarials
    Drug resistance
    Malaria
    Plasmodium falciparum
    Plasmodium malariae
     Plasmodium ovale
     Plasmodium vivax
        (Substituted tetracycline compds. for the treatment of malaria)
IT
    Sulfonamides
    RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (Substituted tetracycline compds. for the treatment of malaria)
ΙT
    Headache
        (and malaise, supplementary compd. for treatment of; Substituted
        tetracycline compds. for the treatment of malaria)
ΙT
    Antimicrobial agents
        (antimicrobial Gram-pos. activity; Substituted tetracycline compds. for
        the treatment of malaria)
ΙT
    Drug delivery systems
        (prodrugs; Substituted tetracycline compds. for the treatment of
        malaria)
ΙT
    Spleen, disease
        (splenomegaly, supplementary compd. for treatment of; Substituted
        tetracycline compds. for the treatment of malaria)
ΙT
    Anemia (disease)
     Fever and Hyperthermia
        (supplementary compd. for treatment of; Substituted tetracycline
        compds. for the treatment of malaria)
IT
    Antipyretics
        (supplementary compd.; Substituted tetracycline compds. for the
        treatment of malaria)
ΙT
    Drug delivery systems
        (tetracycline derivs. for malaria treatment)
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        (Substituted tetracycline compds. for the treatment of malaria)
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    90-34-6, Primaguine
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    RL: BSU (Biological study, unclassified); PAC (Pharmacological activity);
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374748-06-8

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459810-03-8 459810-06-1
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473973-34-1
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473973-64-7
              473973-69-2
                             473973-86-3
                                           473973-96-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
   (Substituted tetracycline compds. for the treatment of malaria)
473974-12-8
              473974-75-3
                             473974-76-4
                                           473974-77-5
                                                          473974-79-7
                             473974-82-2
473974-80-0
              473974-81-1
                                           473974-83-3
                                                          473974-84-4
473974-85-5
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
(Biological study); USES (Uses)
   (Substituted tetracycline compds. for the treatment of malaria)
263760-96-9P, 7-Phenylsancycline
                                   263760-99-2P
                                                   389140-02-7P
389623-67-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
   (tetracycline derivs. for malaria treatment)
98-80-6, Phenylboronic acid 1679-18-1; 4-Chlorophenylboronic acid
                                         14047-29-1, p-Carboxyphenylboronic
1765-93-1, 4-Fluorophenylboronic acid
       35037-73-1, 4-Trifluoromethoxyphenylisocyanate
                                                         59046-78-5
```

TT

IT

IΤ

```
263761-01-9
                   389140-05-0
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (tetracycline derivs. for malaria treatment)
TΤ
     113164-67-3P, 7-Iodosancycline 389140-04-9P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (tetracycline derivs. for malaria treatment)
ΙT
     389623-89-6
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (Substituted tetracycline compds. for the treatment of malaria)
RN
     389623-89-6 HCAPLUS
     2-Naphthacenecarboxamide, 7-(cyclohexylethynyl)-4-(dimethylamino)-
CN
     1, 4, 4a, 5, 5a, 6, 11, 12a-octahydro-3, 10, 12, 12a-tetrahydroxy-1, 11-dioxo-,
     (4S, 4aS, 5aR, 12aS) - (9CI) (CA INDEX NAME)
```

Absolute stereochemistry.

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ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2003 ACS
L12
     2002:716234
                 HCAPLUS
ΑN
DN
     137:247552
ΤI
     Preparation of 7, 9-substituted tetracycline derivatives for
     pharmaceutical use as antibacterial agents
     Nelson, Mark L.; Frechette, Roger; Viski,
ΙN
     Peter; Ismail, Mohamed; Bowser, Todd;
     McIntyre, Laura; Bhatia, Beena; Hawkins, Paul;
     Reddy, Laxma; Stapleton, Karen; Warchol, Tad; Sheahan,
     Paul
PA
     Paratek Pharmaceuticals, Inc., USA
SO
     PCT Int. Appl., 54 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
IC
     ICM C07C237-26
     ICS A61K031-65
     26-6 (Biomolecules and Their Synthetic Analogs)
CC
     Section cross-reference(s): 1, 10, 63
FAN.CNT 1
     PATENT NO.
                            DATE
                                           APPLICATION NO.
                                                            DATE
                      KIND
                                           ______
PΙ
     WO 2002072532
                            20020919
                                           WO 2001-US20722 20010629
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            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,
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RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US 2002193354 A1 20021219 US 2001-895797 20010629

PRAI US 2001-275620P P 20010313

OS MARPAT 137:247552

7,9-Substituted tetracycline derivs., such as I [X = CHC(R13Y'Y), CR6'R6,AΒ S, NR6, O; R2, R2', R4', R4" = H, alkyl, alkenyl, alkynyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, arylalkyl, aryl, heterocyclic, heteroarom., prodrug; R4 = NR4'R4", alkyl, alkenyl, alkynyl, OH, halogen, H; R2', R3, R10, R11, R12 = H, prodrug; R5 = OH, H, thiol, alkanoyl, aroyl, aryl, alkoxy, alkylthio, carbonyloxy; R6, R6' = H, methylene, absent, OH, halogen, thiol, alkyl, alkenyl, alkynyl, alkoxy; R7 = NO2, alkyl, alkenyl, alkynyl, aryl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, amino, arylalkyl, arylalkenyl, arylalkynyl, aminoalkyl; R8 = H, OH, halogen, thiol, alkyl, alkenyl, alkynyl, aryl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl; R9 = NO2, alkyl, alkenyl, alkynyl, aryl, alkoxy; R13 = H, OH, alkyl, alkenyl, alkynyl, aryl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl; Y, Y' = H, halogen, OH, CN, sulfhydryl, amino, alkyl, alkenyl, alkynyl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino], and pharmaceutically acceptable salts thereof, were prepd. to treat numerous tetracycline compd.-responsive states, such as bacterial infections and neoplasms, as well as other known applications for minocycline compds. in general, such as blocking tetracycline efflux and modulation of gene expression. Thus, reaction between N-iodosuccinimide and sancycline hydrochloride hemihydrate yielded 7,9-diiodosancycline II (R = I) which was reacted with 3,4-methylenedioxyphenyl boronic acid to afford 7,9-bis(3,4methylenedioxyphenyl)-sancycline II (R = 3,4-methylenedioxyphenyl). prepd. tetracycline derivs. were tested for antibacterial activity against Staphylococcus aureus, Enterococcus hirae and Escherichia coli.

ST tetracycline deriv prepn antibacterial; sancycline deriv prepn antibacterial

IT Infection

(bacterial, treatment; prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

IT Human

GΙ

(prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

IT Tetracyclines

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents)

```
ΙT
    Escherichia coli
        (prepn. of 7, 9-substituted tetracycline derivs. for treating bacterial
        infection assocd. with E. coli)
     Enterococcus faecalis
IT
        (prepn. of 7, 9-substituted tetracycline derivs. for treating bacterial
        infection assocd. with E. faecalis)
IT
     Enterococcus hirae
        (prepn. of 7, 9-substituted tetracycline derivs. for treating bacterial
        infection assocd. with E. hirae)
IT
     Staphylococcus aureus
        (prepn. of 7, 9-substituted tetracycline derivs. for treating bacterial
        infection assocd. with S. aureus)
TT
     459810-04-9P
                    459810-08-3P
    RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
    preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use
        as antibacterial agents)
                                                459809-44-0P
IT
     330627-26-4P
                    459809-42-8P 459809-43-9P
     459809-45-1P 459809-46-2P 459809-47-3P
                    459809-49-5P
                                   459809-50-8P 459809-51-9P
     459809-48-4P
     459809-52-0P
                    459809-53-1P 459809-54-2P
                                                459809-55-3P
     459809-56-4P
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                                                459809-59-7P
     459809-61-1P 459809-63-3P 459809-65-5P
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                    459810-07-2P 459810-09-4P
                                                459810-11-8P
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use
        as antibacterial agents)
IT
     516-12-1, N-Iodosuccinimide
                                   808-26-4, Sancycline
                                                           1066-54-2,
     Trimethylsilyl acetylene
                                50696-61-2, Cyclohexenyl-acetylene
                                                                      53173-80-1
     94839-07-3, 3,4-Methylenedioxyphenyl boronic acid
                                                         389625-14-3
     459810-12-9
                   460091-55-8, Sancycline hydrochloride hemihydrate
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use
        as antibacterial agents)
     113164-67-3P, 7-Iodosancycline 263761-05-3P, 7-Ethynylsancycline
    263761-08-6P, 7,9-Diiodosancycline 389624-14-0P,
     7-Ethylsancycline 459810-10-7P
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use
        as antibacterial agents)
RE.CNT
              THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Ashley, R; WO 0028983 A 2000 HCAPLUS
(2) Farmaceutici Italia; DE 2346535 A 1974 HCAPLUS
(3) Farmaceutici Italia; DE 2527568 A 1976 HCAPLUS
(4) James, H; US 3338963 A 1967 HCAPLUS
(5) Winterbottom, R; US 3433834 A 1969 HCAPLUS
IT
    459810-04-9P
    RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
    preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (prepn. of 7, 9-substituted tetracycline derivs. for pharmaceutical use
```

as antibacterial agents)

RN 459810-04-9 HCAPLUS

2-Naphthacenecarboxamide, 4-(dimethylamino)-7-ethyl-1,4,4a,5,5a,6,11,12a-CN octahydro-3,10,12,12a-tetrahydroxy-9-iodo-1,11-dioxo-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

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L12 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2003 ACS
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2002:716035 HCAPLUS ΑN

DN 137:244598

Substituted tetracycline compounds as synergistic antifungal agents ΤI

Draper, Michael; Nelson, Mark L. IN

PΑ Paratek Pharmaceuticals, Inc., USA

PCT Int. Appl., 114 pp. SO

CODEN: PIXXD2

DTPatent

LA English

IC ICM A61K

10-5 (Microbial, Algal, and Fungal Biochemistry) CC Section cross-reference(s): 1, 5, 26

FAN.CNT 1

	PATENT NO.				KII	ND	DATE			A.	PPLI	CATI	N NC	ο.	DATE					
ΡI	WO	2002	0720	31	A2 20020919					M	20°	02-U	S782	9	20020314					
		W:	ΑE,	AG,	AL,	AM,	AT,	ΑU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,		
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,		
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	ΝZ,	OM,	PH,		
			PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,		
			UA,	UG,	UZ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM	
		RW:	GH,	GM,	KE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	CH,		
			CY,	DE,	DK,	ES,	FΙ,	FR,	GB,	GR,	ΙE,	ΙΤ,	LU,	MC,	NL,	PT,	SE,	TR,		
			BF,				CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	ΤG		
PRAI	US	2001	001-275899P P 20010314																	

PRAI US 2001-275899P

OS MARPAT 137:244598

Methods and compns. for treating for the synergistic treatment of fungal AB assocd. disorders are discussed. The method includes administering the antifungal agent with an effective amt. of a substituted tetracycline compd., such that the antifungal activity of the antifungal agent is increased. Examples of antifungal agents include polyenes such as amphotericin B.

ST tetracycline synergistic antifungal agent

ΙT Actinomyces

(actinomycosis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

IT Aspergillus

(aspergillosis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

IT Blastomyces Mycosis

(blastomycosis, North American; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) Blastomyces Mycosis (blastomycosis; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) Candida albicans

ΙT

(candidiasis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT Drug delivery systems

> (carriers; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

TΤ Skin, disease

> (chromoblastomycosis; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

IT Mycosis

IT

(coccidioidomycosis; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT Tinea (skin disease)

> (cruris; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT Cryptococcus neoformans

> (cryptococcosis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT Lymphatic system

> (disease, epizootic lymphangitis; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT Toxicity

(drug, immunosuppression from, fungal infections in; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT Entomophthorales

> (entomophthoromycosis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ITHistoplasma farciminosum

(epizootic lymphangitis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT Immunosuppression

> (from chemotherapy, fungal infections in; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT AIDS (disease)

Immunodeficiency

(fungal infections in; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT Disease, plant

(fungal; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT Geotrichum candidum

> (geotrichosis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

IT Chemotherapy

> (immunosuppression from, fungal infections in; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

IT Histoplasma capsulatum

(infection with; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT Skin-infecting fungi

(infections from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

ΙT

(mucormycosis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

IT Mycosis

Service of

(mycetoma; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) IT Oomycetes (oomycosis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) IT Paecilomyces (paecilimycosis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) ΙT Paracoccidioides brasiliensis (paracoccidioidomycosis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) IT Penicillium (penicilliosis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) IT (rhinosporidiosis from; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) ΙT Aspergillus nidulans Athlete's foot Candida albicans Candida dubliniensis Candida glabrata Candida guilliermondii Candida krusei Candida lusitaniae Candida neoformans Candida parapsilosis Candida tropicalis Cytotoxicity Human Issatchenkia orientalis Mammalia Mvcosis (substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) TT Polyenes Tetracyclines RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) Drug interactions IT Fungicides (synergistic; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) IT Anti-inflammatory agents (tetracyclines; substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) ΙT 389624-44-6P RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity) 263761-05-3P 351336-94-2P 380435-63-2P 389623-77-2P 389624-48-0P 389624-49-1P 389624-67-3P 460068-27-3P 460069-92-5P 460072-21-3P 389624-88-8P 460073-43-2P 460073-62-5P 460073-68-1P 460073-05-6P 460073-82-9P 460074-13-9P 460074-36-6P 460074-56-0P 460074-58-2P 460074-69-5P RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological

activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL

```
(Biological study); PREP (Preparation); USES (Uses)
        (substituted tetracycline compds. as synergistic antifungal agents in
        relation to cytotoxicity)
ΙT
     564-25-0
                                             5995-55-1
                1397-89-3, Amphotericin B
                                                          31642-30-5
                                                                        35689-65-7
     113164-67-3
                                  146253-75-0
                                                 146278-03-7
                                                               151922-17-7
                   120793-45-5
     161321-34-2
                                                               186759-53-5
                   161452-36-4
                                  186759-47-7
                                                 186759-51-3
                   220620-09-7
                                  233585-94-9
                                                 233585-95-0
                                                               233586-04-4
     186759-61-5
                   233586-11-3
                                                 263760-96-9
     233586-06-6
                                  233586-12-4
                                                               263760-99-2
                   263761-08-6
                                                 295356-12-6
     263761-02-0
                                  295356-11-5
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     activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (substituted tetracycline compds. as synergistic antifungal agents in
        relation to cytotoxicity)
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RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological
activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
   (substituted tetracycline compds. as synergistic antifungal agents in
   relation to cytotoxicity)
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N'-Benzyl-N, N-dimethylethylenediamine 103-76-4, 1-Piperazineethanol 111-30-8, Glutaraldehyde 122-78-1, Phenylacetaldehyde 622-77-5, 808-26-4, Sancycline 871-84-1, 1,7-Octadiyne Benzylcyanamide 27329-70-0, 2-Formylfuran-5-boronic 914-00-1, Methacycline 4199-35-3 50696-61-2, Cyclohexenylacetylene 55552-70-0, 3-Furanylboronic acid 107099-99-0, 2,5-Dimethoxyphenylboronic acid 128796-39-4, 4-Trifluoromethylphenylboronic acid 144025-03-6, 2,4-Difluorophenylboronic acid 149104-90-5 380435-62-1 149934-19-0 460076-33-9 460076-36-2 389140-04-9 **459810-03-8** 460076-37-3

RL: RCT (Reactant); RACT (Reactant or reagent) (substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

IT 460076-34-0P 460076-35-1P 460076-38-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

IT 389624-44-6P

TΨ

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(substituted tetracycline compds. as synergistic antifungal agents in relation to cytotoxicity)

RN 389624-44-6 HCAPLUS

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-(1-propynyl)-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

- L12 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2003 ACS
- AN 2002:716027 HCAPLUS
- DN 137:244597
- TI Substituted tetracycline compounds as antifungal agents
- IN Draper, Michael; Nelson, Mark L.
- PA Paratek Pharmaceuticals, Inc., USA
- SO PCT Int. Appl., 71 pp. CODEN: PIXXD2
- DT Patent
- LA English

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IC
     ICM A61K
     10-5 (Microbial, Algal, and Fungal Biochemistry)
CC
     Section cross-reference(s): 1, 5, 26
FAN.CNT 1
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                      KIND DATE
                                          APPLICATION NO. DATE
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     _____
                                      WO 2002-US7502 20020314
    WO 2002072022
                     A2 20020919
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             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
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                            20010314
PRAI US 2001-275948P
    MARPAT 137:244597
OS
    Methods and compns. for treating fungal assocd. disorders in subjects are
AB
     discussed. The method includes contacting the fungus with an effective
     amt. of a substituted tetracycline compd., such that the growth of said
     fungus is inhibited.
ST
     tetracycline antifungal agent
ΙT
    Actinomyces
        (actinomycosis from; substituted tetracycline compds. as antifungal
        agents in relation to cytotoxicity)
ΙT
        (agrochem.; substituted tetracycline compds. as antifungal agents in
        relation to cytotoxicity)
ΙT
    Aspergillus
        (aspergillosis from; substituted tetracycline compds. as antifungal
        agents in relation to cytotoxicity)
ΙT
     Blastomyces
    Mycosis
        (blastomycosis, North American; substituted tetracycline compds. as
        antifungal agents in relation to cytotoxicity)
ΙT
     Blastomyces
    Mycosis
        (blastomycosis; substituted tetracycline compds. as antifungal agents
        in relation to cytotoxicity)
ΙT
     Candida albicans
        (candidiasis from; substituted tetracycline compds. as antifungal
        agents in relation to cytotoxicity)
IT
     Drug delivery systems
        (carriers; substituted tetracycline compds. as antifungal agents in
        relation to cytotoxicity)
ΙT
     Skin, disease
        (chromoblastomycosis; substituted tetracycline compds. as antifungal
        agents in relation to cytotoxicity)
ΙT
     Mycosis
        (coccidioidomycosis; substituted tetracycline compds. as antifungal
        agents in relation to cytotoxicity)
ΙT
     Tinea (skin disease)
        (cruris; substituted tetracycline compds. as antifungal agents in
        relation to cytotoxicity)
ΙT
     Cryptococcus neoformans
        (cryptococcosis from; substituted tetracycline compds. as antifungal
        agents in relation to cytotoxicity)
ΙT
     Lymphatic system
        (disease, epizootic lymphangitis; substituted tetracycline compds. as
        antifungal agents in relation to cytotoxicity)
ΙT
     Toxicity
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(drug, immunosuppression from, fungal infections in; substituted

tetracycline compds. as antifungal agents in relation to cytotoxicity) ΙT Entomophthorales (entomophthoromycosis from; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) ΙT Histoplasma farciminosum (epizootic lymphangitis from; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) ΙT Immunosuppression (from chemotherapy, fungal infections in; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) AIDS (disease) ΙT Immunodeficiency (fungal infections in; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) IT Disease, plant (fungal; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) ΙT Geotrichum candidum (geotrichosis from; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) ΙT Chemotherapy (immunosuppression from, fungal infections in; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) ΙT Histoplasma capsulatum (infection with; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) IT Skin-infecting fungi (infections from; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) ΙT Mucor (mucormycosis from; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) IT Mycosis (mycetoma; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) ΙT Oomycetes (oomycosis from; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) ΙT Paecilomyces (paecilimycosis from; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) Paracoccidioides brasiliensis ΙT (paracoccidioidomycosis from; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) IT Penicillium (penicilliosis from; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) ΙT Rhinosporidium (rhinosporidiosis from; substituted tetracycline compds. as antifungal agents in relation to cytotoxicity) ΙT Athlete's foot Candida Candida albicans Candida dubliniensis Candida glabrata Candida quilliermondii Candida krusei Candida lusitaniae Candida neoformans Candida parapsilosis Candida tropicalis Cytotoxicity

Fungicides

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Human
    Mammalia
    Mycosis
        (substituted tetracycline compds. as antifungal agents in relation to
        cytotoxicity)
IT
    Tetracyclines
    RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological
     activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (substituted tetracycline compds. as antifungal agents in relation to
        cytotoxicity)
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     activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (a csubstituted tetracycline compds. as antifungal agents in relation
        to cytotoxicity)
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     460071-99-2
     460073-37-4 460073-68-1
                               460074-28-6
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                                               460082-77-3
                                                              460082-81-9
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                                               460082-85-3 460082-86-4
     460082-87-5
                   460082-88-6
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                                               460082-90-0
                                                              460082-91-1
    RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological
    activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (substituted tetracycline compds. as antifungal agents in relation to
        cytotoxicity)
ΙT
     693-02-7, 1-Hexyne
                          808-26-4, Sancycline
                                                 85199-06-0,
     2,5-Dimethylphenylboronic acid
                                      389139-46-2, 9-(4-
    Fluorophenylethynyl)minocycline
                                       389140-04-9
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (substituted tetracycline compds. as antifungal agents in relation to
        cytotoxicity)
     389139-70-2P, 9-(4'-Fluorophenylethyl)-Minocycline
ΙT
                                                           460082-93-3P
     460082-94-4P, 9-(2',5'-Dimethylphenyl)minocycline
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (substituted tetracycline compds. as antifungal agents in relation to
        cytotoxicity)
IT
     389623-86-3
     RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological
     activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (substituted tetracycline compds. as antifungal agents in relation to
        cytotoxicity)
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RN 389623-86-3 HCAPLUS
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CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-(phenylethynyl)-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

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L12 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2003 ACS
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AN 2002:51420 HCAPLUS

DN 136:102232

TI Preparation of 7-substituted tetracycline derivatives for pharmaceutical use as antibacterial agents

IN Nelson, Mark L.; Frechette, Roger; Viski,
 Peter; Ismail, Mohamed; Bowser, Todd;
 Bhatia, Beena; Messersmith, David; McIntyre,
 Laura; Koza, Darrell; Rennie, Glen; Sheahan,
 Paul; Hawkins, Paul; Verma, Atul; Warchol,
 Tad; Bandarage, Upul

PA Trustees of Tufts College, USA; Paratek Pharmaceuticals, Inc.

SO PCT Int. Appl., 97 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07C237-00

CC 26-6 (Biomolecules and Their Synthetic Analogs)
 Section cross-reference(s): 10

FAN.CNT 1

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ΡΙ				-	A2 A3					WO 2001-US20766 20010629									
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			•	•								-			NO, TZ,			•	
		RW:		,	,	,	AM, MW	•	•	•	•				TM AT,	BE.	СН	CY	
		100.	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	•	•	
			0550	25 ·	A1 2003			0320	,	GN, GW, ML, MR, NE, SN, TD, TG US 2001-895812 20010629									
	EΡ	7 1301466 R: AT, BE,																PT.	
DDAT			ΙE,	SI,	LT,	LV,	FI,	RO,					,		•	·	•	,	
PRAI	US	2000 2001	-275	576P	Р		2001	0313											
os		2001 RPAT					2001	0629											
CT											•								

GI

7-Substituted tetracycline derivs., such as I [R7 = NO2, alkyl, alkenyl, AB alkynyl, aryl, alkoxy, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, arylalkyl, amino, arylalkenyl, arylalkynyl, aminoalkyl, etc.], were prepd. for therapeutic use as antibacterial agents. Thus, 7-phenylsancycline I (R7 = Ph) was prepd. in 42% yield by arom. coupling reaction of 7-iodosancycline I (R7 = iodo) with PhB(OH)2 using Pd(OAc)2 and Na2CO3 in MeOH under an argon atm. at r.t. for 2 h. The prepd. tetracycline derivs. were tested for antibacterial activity against Escherichia coli, Enterococcus hirae, and Staphylococcus aureus. ST tetracycline deriv prepn antibacterial agent; sancycline deriv prepn antibacterial agent ΙT Antibacterial agents (prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents) IΤ 263761-01-9P 389624-24-2P 389624-36-6P RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as antibacterial agents) ΙT 263760-96-9P 263760-98-1P 263760-99-2P 263761-02-0P 365277-42-5P 365277-44-7P 365277-45-8P 374748-06-8P 380435-62-1P 380435-63-2P 380435-65-4P 380435-76-7P 389623-67-0P 389623-72-7P 389623-74-9P 389623-77-2P 389623-80-7P 389623-82-9P 389623-84-1P 389623-88-5P 389623-89-6P 389623-86-3P 389623-90-9P 389623-91-0P 389623-93-2P 389623-95-4P 389623-97-6P 389623-98-7P 389623-99-8P 389623-96-5P 389624-00-4P 389624-01-5P 389624-02-6P 389624-05-9P 389624-06-0P 389624-03-7P 389624-04-8P 389624-07-1P **389624-08-2P 389624-09-3P** 389624-13-9P 389624-10-6P 389624-11-7P 389624-12-8P 389624-14-0P 389624-15-1P 389624-16-2P 389624-17-3P 389624-18-4P 389624-19-5P 389624-21-9P 389624-22-0P 389624-23-1P 389624-20-8P 389624-25-3P 389624-26-4P 389624-27-5P 389624-29-7P 389624-30-0P 389624-31-1P 389624-28-6P 389624-32-2P 389624-33-3P 389624-34-4P 389624-35-5P 389624-37-7P 389624-38-8P 389624-39-9P 389624-40-2P 389624-41-3P 389624-42-4P 389624-43-5P 389624-44-6P 389624-45-7P **389624-46-8P 389624-47-9P** 389624-48-0P 389624-49-1P 389624-50-4P 389624-51-5P 389624-52-6P 389624-53-7P 389624-54-8P 389624-55-9P **389624-56-0P** 389624-57-1P 389624-58-2P 389624-59-3P **389624-60-6P 389624-61-7P** 389624-62-8P 389624-63-9P 389624-64-0P 389624-65-1P 389624-66-2P 389624-67-3P 389624-68-4P 389624-69-5P **389624-70-8P** 389624-71-9P 389624-72-0P 389624-73-1P

389624-74-2P 389624-75-3P 389624-76-4P

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                                                                  389625-13-2P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
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        (prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as
        antibacterial agents)
ΙT
     98-80-6
               623-47-2
                          808-26-4
                                     871-84-1, 1,7-Octadiyne
     1679-18-1
                 1765-93-1
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                                         7223-38-3
                                                      93501-84-9
                                                                   127972-02-5
     389625-14-3
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as
        antibacterial agents)
ΙT
     113164-67-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as
        antibacterial agents)
     389624-36-6P
ΙT
    RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic
    preparation); THU (Therapeutic use); BIOL (Biological study); PREP
     (Preparation); RACT (Reactant or reagent); USES (Uses)
        (prepn. of 7-substituted tetracycline derivs. for pharmaceutical use as
        antibacterial agents)
     389624-36-6 HCAPLUS
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     2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-
CN
     3,10,12,12a-tetrahydroxy-7-[(3-methoxyphenyl)ethynyl]-1,11-dioxo-,
     (4S, 4aS, 5aR, 12aS) - (9CI) (CA INDEX NAME)
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Absolute stereochemistry.

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L12 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2003 ACS
AN 2002:51417 HCAPLUS
DN 136:102229
TI Preparation of 7,8 and 9-substituted tetracycline derivatives
IN Nelson, Mark L.; Koza, Darrell
PA Trustees of Tufts College, USA
SO PCT Int. Appl., 26 pp.
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LA
     English
IC
     ICM C07C237-00
CC
     26-6 (Biomolecules and Their Synthetic Analogs)
     Section cross-reference(s): 1, 10, 63
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     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                             DATE
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PRAI US 2000-216656P
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                            20010629
OS
    MARPAT 136:102229
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CODEN: PIXXD2

Patent

DT

The 7,8 and 9-substituted tetracycline derivs. I (Rl = H, OH; R2, R3 = H, Me, OH; R4 = H, alkenyl, alkynyl, Ph, halophenyl, acyl, phenylalkynyl, heteroaryl, dimethylamino: R5 = H, Ph, nitrophenyl, halo, alkynyl; R6 = H, amino, acetamide, alkynyl; at least one of R4, R5, and R6 is not H) and their pharmaceutically acceptable salts were as antibacterial agents. Thus, tetracycline underwent iodination with NIS to give a mixt. of 7- and 9-iodotetracycline, of which the 7- isomer was treated AsPh3 in presence of Pd(PPh3)2Cl2 and CuI to give 7-phenyltetracycline. I were screened to detn. their in vitro antibacterial min. inhibitory concn. (no data).

Ι

ST tetracycline substituted prepn antibacterial

IT Antibacterial agents

Antibiotics

(prepn. of 7.8 and 9-substituted tetracycline derivs. as antibacterial agents)

IT **263761-03-1P** 295356-13-7P 295356-15-9P 295356-16-0P

295356-17-1P 330627-27-5P 389139-16-6P 389570-43-8P 389570-44-9P

389570-45-0P 389570-46-1P 389570-48-3P 389570-49-4P

389570-50-7P 389570-51-8P 389570-52-9P **389570-53-0P**

389570-54-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 7,8 and 9-substituted tetracycline derivs. as antibacterial agents)

IT 60-54-8, Tetracycline 10592-13-9, Doxycycline hydrochloride

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of 7,8 and 9-substituted tetracycline derivs. as antibacterial agents)

IT 120793-45-5P 161321-34-2P 295356-11-5P 295356-12-6P 330627-20-8P 389570-41-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 7,8 and 9-substituted tetracycline derivs. as antibacterial agents)

IT 389570-42-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(prepn. of 7,8 and 9-substituted tetracycline derivs. as antibacterial agents)

IT 263761-03-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 7,8 and 9-substituted tetracycline derivs. as antibacterial agents)

RN 263761-03-1 HCAPLUS

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-ethenyl-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

- L12 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2003 ACS
- AN 2001:208235 HCAPLUS
- DN 134:252206
- TI Methods of preparing substituted tetracyclines with transition metal-based chemistries
- IN Nelson, Mark L.; Rennie, Glen; Koza, Darrell
- PA Trustees of Tufts College, USA
- SO PCT Int. Appl., 46 pp.

CODEN: PIXXD2

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DT
     Patent
LA
     English
     ICM C07C237-26
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     ICS C07C231-12; A61K031-65; A61P031-04
     26-6 (Biomolecules and Their Synthetic Analogs)
CC
     Section cross-reference(s): 10
FAN.CNT 9
                                            APPLICATION NO.
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     WO 2001019784
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             HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
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PRAI US 1999-154701P
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     WO 2000-US25040
     CASREACT 134:252206; MARPAT 134:252206
OS
GΙ
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AB Substituted tetracyclinrderivs. were prepd. by combining a reactive tetracycline-based precursor and a reactive org. substituent precursor in

Ι

 $x = (x + x, y) \cdot x = x^{-\alpha}$

the presence of a transition metal catalyst. In one embodiment of the invention, a substituted tetracycline compd. may be prepd. by combining a reactive tetracycline-based precursor compd. such as an arene tetracycline diazonium salt, and a reactive org. substituent precursor, e.g., alkenes, substituted alkenes, vinyl monomers, aroms. and heteroaroms., in the presence of a transition metal catalyst, such as palladium chloride, under conditions such that a tetracycline compd. substituted with the org. substituent is formed. Such compds. may optionally act as intermediates for making other compds., e.g., hydrogenation of unsatd. groups on the substituent. Thus, sancycline-HCl was treated with N-iodosuccinimide in concd. H2SO4 to give 61% 7-iodosancycline and 22% 7,9-diodosancycline. 7-Iodosancycline was added to a degassed soln. of MeOH contg. Na2CO3 and Pd(OAc)2 and then 4-chlorophenylbroonic added to give 7-(4-chlorophenyl)sancycline (I). Antibacterial activity of several derivs. was tabulated.

- ST tetracycline deriv prepn transition metal chem; antibacterial tetracycline deriv
- IT Tetracyclines

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(methods of prepg. substituted tetracyclines with transition metal-based chemistries)

- IT Transition metals, uses
 - RL: CAT (Catalyst use); USES (Uses)

(organopalladium catalysts; methods of prepg. substituted tetracyclines with transition metal-based chemistries)

IT 330627-29-7 330627-30-0 330627-31-1 330627-32-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(methods of prepg. substituted tetracyclines with transition metal-based chemistries)

IT 263760-99-2P 330627-21-9P 330627-22-0P 330627-26-4P 344771-54-6P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); IMF (Industrial manufacture); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(methods of prepg. substituted tetracyclines with transition metal-based chemistries)

IT 3375-31-3 7447-39-4, Cupric chloride, uses 7647-10-1, Palladium chloride 13767-71-0, Cupric iodide 13965-03-2, Bistriphenylphosphinedichloropalladium 14220-64-5, Bisbenzonitriledichloropalladium 15956-28-2, Rhodium (II) acetate

51364-51-3 143006-99-9 RL: CAT (Catalyst use); USES (Uses)

(methods of prepg. substituted tetracyclines with transition metal-based chemistries)

IT 113164-67-3P 120793-45-5P 161321-34-2P 330627-20-8P 330627-23-1P 330627-25-3P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (methods of prepg. substituted tetracyclines with transition metal-based chemistries)

IT 263760-98-1P 263761-01-9P **263761-03-1P** 263761-08-6P 330627-24-2P 330627-27-5P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(methods of prepg. substituted tetracyclines with transition metal-based chemistries)

TT 57-62-5 79-10-7, Propenoic acid, reactions 79-57-2, Oxytetracycline 98-80-6, Phenylboronic acid 100-42-5, Styrene, reactions 127-33-3, Demeclocycline 141-32-2, Butyl acrylate 564-25-0, Doxycycline 751-97-3, Rolitetracycline 808-26-4, Sancycline 914-00-1, Methacycline 992-21-2, Lymecycline 1110-80-1, Pipacycline 1679-18-1, 4-Chlorophenylboronic acid 1765-93-1, 4-Fluorophenylboronic acid

4363-34-2, Etheneboronic acid 4599-60-4, Penimepicycline 6625-20-3, Sancycline hydrochloride 10118-90-8, Minocycline 10592-13-9, 15590-00-8, Etamocycline Doxycycline hydrochloride 15599-51-6, Apicycline 16259-34-0, Penimocycline 16545-11-2, Guamecycline 24067-17-2, 4-Nitrophenylboronic acid 29144-42-1, Chelocardin 31770-79-3, Meglucycline 149934-19-0 197958-29-5, 2-Pyridylboronic RL: RCT (Reactant); RACT (Reactant or reagent) (methods of prepg. substituted tetracyclines with transition metal-based chemistries) 171807-99-1P

TT

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(methods of prepg. substituted tetracyclines with transition metal-based chemistries)

RE.CNT THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD

- (1) Ahmad, N; JOUR CHEM SOC PAK 1990, V12(2), P168 HCAPLUS
- (2) Koza, D; ORGANIC LETTERS 2000, V2(6), P815 HCAPLUS

IT 263761-03-1P

> RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(methods of prepg. substituted tetracyclines with transition metal-based chemistries)

RN 263761-03-1 HCAPLUS

2-Naphthacenecarboxamide, 4-(dimethylamino)-7-ethenyl-1,4,4a,5,5a,6,11,12a-CN octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

- L12 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2003 ACS
- ΑN 2000:137899 HCAPLUS
- DN 132:279036
- TΙ Synthesis of 7-Substituted Tetracycline Derivatives
- ΑU Koza, Darrell J.
- Department of Science and Allied Health, Mount Ida College, Newton, MA, CS 02459, USA
- SO Organic Letters (2000), 2(6), 815-817 CODEN: ORLEF7; ISSN: 1523-7060
- PB American Chemical Society
- DT Journal
- English LA
- CC 26-6 (Biomolecules and Their Synthetic Analogs)
- The synthesis of 7-substituted tetracycline derivs. has been accomplished AB in high yield from 7-halotetracyclines by modified Suzuki and Stille coupling protocols. These novel derivs. may serve as a new class of tetracycline antibiotics effective against multi-antibiotic-resistant bacteria.
- ST tetracycline deriv synthesis; sancycline deriv synthesis

```
TΤ
    Stille coupling reaction
    Suzuki coupling reaction
        (synthesis of 7-substituted tetracycline derivs.)
IT
     Tetracyclines
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis of 7-substituted tetracycline derivs.)
IT
     98-80-6, Phenylboronic acid
                                  960-16-7, Phenyltributyltin
                                                                 994-89-8,
                          6625-20-3, Sancycline hydrochloride
                                                                7486-35-3,
    Ethynyltributyltin
    Vinyltributyltin
                        17151-47-2, (4-Fluorophenyl)tributyltin
     (4-Chlorophenyl) tributyltin
                                  28611-39-4, (4-Dimethylaminophenyl)boronic
            79048-32-1, (4-Nitrophenyl)tributyltin
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (synthesis of 7-substituted tetracycline derivs.)
    113164-67-3P, 7-Iodosancycline
ΙT
    RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (synthesis of 7-substituted tetracycline derivs.)
ΙT
    263760-96-9P
                    263760-98-1P
                                   263760-99-2P
                                                  263761-01-9P
                                                                 263761-02-0P
    263761-03-1P 263761-05-3P
                                 263761-08-6P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis of 7-substituted tetracycline derivs.)
RE.CNT
              THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Beereboom, J; J Am Chem Soc 1960, V82, P1003 HCAPLUS
(2) Boothe, J; J Am Chem Soc 1960, V82, P1253 HCAPLUS
(3) Broschard, R; Science 1949, V109, P199 HCAPLUS
(4) Brown, A; J Chem Soc, Perkin Tran 1992, V1, P123
(5) Buchwald, S; J Am Chem Soc 1998, V120, P9722
(6) Finlay, A; Science 1950, V111, P85 HCAPLUS
(7) Hlavka, J; J Am Chem Soc 1962, V84, P1426 HCAPLUS
(8) McCormick, J; Antibiot Ann 1953, P81
(9) Mitscher, L; The Chemistry of Tetracycline Antibiotics 1978, V9 HCAPLUS
(10) Nicolaou, K; Tetrahedron Lett 1998, V39, P7665
(11) Pattenden, G; Synth Lett 1993, P215 HCAPLUS
(12) Petisi, J; J Med Chem 1962, V5, P538 HCAPLUS
(13) Redin, G; Antimicrob Agents Chemother 1966, P371 HCAPLUS
(14) Stille, J; Angew Chem, Int Ed Engl 1986, V25, P508
(15) van Honweling, C; F D A Papers 1969, P21
IT
    263761-03-1P
    RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis of 7-substituted tetracycline derivs.)
    263761-03-1 HCAPLUS
RN
    2-Naphthacenecarboxamide, 4-(dimethylamino)-7-ethenyl-1,4,4a,5,5a,6,11,12a-
CN
    octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI)
```

Absolute stereochemistry.

(CA INDEX NAME)

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STRUCTURE FILE UPDATES: 27 APR 2003 HIGHEST RN 506405-59-0 DICTIONARY FILE UPDATES: 27 APR 2003 HIGHEST RN 506405-59-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

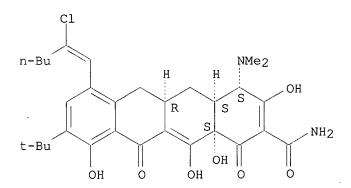
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d 16 ide can 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75 80 85 90 91

- L6 ANSWER 5 OF 91 REGISTRY COPYRIGHT 2003 ACS
- RN 488817-71-6 REGISTRY
- CN 2-Naphthacenecarboxamide, 7-(2-chloro-1-hexenyl)-4-(dimethylamino)-9-(1,1-dimethylethyl)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C31 H39 C1 N2 O7
- SR CA
- LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry. Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 1 REFERENCES IN FILE CA (1957 TO DATE)
- 1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

L6 ANSWER 10 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 488817-66-9 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[2-[4-(trifluoromethyl)phenyl]etheny l]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C30 H27 F3 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

L6 ANSWER 15 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 488817-59-0 REGISTRY

CN 2-Naphthacenecarboxamide, 7-(2-chloro-3-hydroxy-1-propenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H25 C1 N2 O8

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

L6 ANSWER 20 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 488817-25-0 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-ethenyl-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H26 N2 O8

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

L6 ANSWER 25 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 488815-47-0 REGISTRY

CN 2-Propenoic acid, 3-[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]-, 3-(dimethylamino)propyl ester (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H35 N3 O9

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry. Double bond geometry unknown.

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

L6 ANSWER 30 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 460069-76-5 REGISTRY

CN 2-Naphthacenecarboxamide, 7-[(1E)-2-(4-chlorophenyl)ethenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H27 C1 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 137:244598

L6 ANSWER 35 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 459809-43-9 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7,9-bis[(4-methoxyphenyl)ethynyl]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C39 H34 N2 O9

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

2 REFERENCES IN FILE CA (1957 TO DATE)

2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:247552

L6 ANSWER 40 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 389624-78-6 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-(1-pentynyl)-, (4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H28 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1957 TO DATE)

4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:244598

REFERENCE 3: 137:244597

REFERENCE 4: 136:102232

L6 ANSWER 45 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 389624-65-1 REGISTRY

CN 2-Naphthacenecarboxamide, 7-[(12)-2-chloro-1-hexenyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-,(4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H31 C1 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1957 TO DATE)

3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 137:244598

REFERENCE 2: 137:244597

REFERENCE 3: 136:102232

L6 ANSWER 50 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 389624-53-7 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[(1E)-2-[4-(trifluoromethyl)phenyl]ethenyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C30 H27 F3 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

Double bond geometry as shown.

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 137:244598

REFERENCE 2: 136:102232

L6 ANSWER 55 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 389624-46-8 REGISTRY

CN 2-Naphthacenecarboxamide, 7-(3-amino-3-oxo-1-propenyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H25 N3 O8

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry. Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE) 2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 136:102232

L6 ANSWER 60 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 389624-38-8 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(3-methyl-1-pentynyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H30 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1957 TO DATE) 5 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:333118

REFERENCE 3: 137:244598

REFERENCE 4: 137:244597

REFERENCE 5: 136:102232

L6 ANSWER 65 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 389624-27-5 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-(3-pyridinylethynyl)-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H25 N3 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

3 REFERENCES IN FILE CA (1957 TO DATE)

3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:333118

REFERENCE 3: 136:102232

L6. ANSWER 70 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 389624-18-4 REGISTRY

CN 2-Naphthacenecarboxamide, 7-(1-cyclohexen-1-ylethynyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H30 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1957 TO DATE)

5 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:333118

REFERENCE 3: 137:244598

REFERENCE 4: 137:244597

REFERENCE 5: 136:102232

L6 ANSWER 75 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 389624-10-6 REGISTRY

CN 2-Pentenedioic acid, 4-[[(6aS,10S,10aS,11aR)-8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-1-naphthacenyl]methylene]-2-iodo-, diethyl ester, (2Z,4Z)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C31 H33 I N2 O11

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 137:333118

REFERENCE 2: 136:102232

L6 ANSWER 80 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 389624-00-4 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-[(1E)-3-(dimethylamino)-3-oxo-1-propenyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C26 H29 N3 O8

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1957 TO DATE)
2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 137:333118

REFERENCE 2: 136:102232

L6 ANSWER 85 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 389623-89-6 REGISTRY

CN 2-Naphthacenecarboxamide, 7-(cyclohexylethynyl)-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-,(4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H32 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 5 REFERENCES IN FILE CA (1957 TO DATE)
- 5 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:333118

REFERENCE 3: 137:244598

REFERENCE 4: 137:244597

REFERENCE 5: 136:102232

L6 ANSWER 90 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 263761-05-3 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-ethynyl-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN 7-Ethynylsancycline

FS STEREOSEARCH

MF C23 H22 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1957 TO DATE)

3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 137:247552

REFERENCE 2: 137:244598

REFERENCE 3: 132:279036

L6 ANSWER 91 OF 91 REGISTRY COPYRIGHT 2003 ACS

RN 263761-03-1 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-ethenyl-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

DR 330627-28-6

MF C23 H24 N2 O7

SR CA

LC STN Files: CA, CAPLUS, CASREACT, USPATFULL

3 REFERENCES IN FILE CA (1957 TO DATE)

3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 136:102229

REFERENCE 2: 134:252206

REFERENCE 3: 132:279036

=> d 17 ide can 5 10 15 20 25 30 35 40 45 50 55 60 65 70 75

L7 ANSWER 5 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 488820-20-8 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(2-methylpropyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C25 H30 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

L7 ANSWER 10 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 488819-90-5 REGISTRY

CN 2-Naphthacenecarboxamide, 7-acetyl-4-(dimethylamino)-9-[[(2,2-

dimethylpropyl)amino]methyl]-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H37 N3 O8

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

L7 ANSWER 15 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 488818-28-6 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-(4-morpholinyloxoacetyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C27 H29 N3 O10

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

L7 ANSWER 20 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 488817-80-7 REGISTRY

CN 1-Naphthacenepropanoic acid, 8-(aminocarbonyl)-10-(dimethylamino)-5,6a,7,10,10a,11,11a,12-octahydro-4,6,6a,9-tetrahydroxy-5,7-dioxo-, methyl ester, (6aS,10S,10aS,11aR)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C25 H28 N2 O9

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

L7 ANSWER 25 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 460073-66-9 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-9-[[[(4-methoxyphenyl)amino]carbonyl]amino]-7-(1-methylethyl)-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C32 H36 N4 O9

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1957 TO DATE)

1 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 137:244598

L7 ANSWER 30 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 460068-84-2 REGISTRY

CN 2-Naphthacenecarboxamide, 7-acetyl-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,5,10,12,12a-pentahydroxy-6-methyl-1,11-dioxo-, (4S,4aR,5S,5aR,6R,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C24 H26 N2 O9

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1957 TO DATE)

3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:244598

REFERENCE 3: 137:244597

L7 ANSWER 35 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 459809-99-5 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-9-(1,1-dimethylethyl)1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-7-[(1Z)-1(methoxyimino)ethyl]-1,11-dioxo-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H35 N3 O8

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

Double bond geometry as shown.

4 REFERENCES IN FILE CA (1957 TO DATE)

4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 137:333118

2: 137:247552 REFERENCE

REFERENCE 137:244598 3:

REFERENCE 4: 137:244597

ANSWER 40 OF 75 REGISTRY COPYRIGHT 2003 ACS L7

RN 459809-67-7 REGISTRY

CN 2-Naphthacenecarboxamide, 7,9-diacetyl-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-, (4S, 4aS, 5aR, 12aS) - (9CI) (CA INDEX NAME)

STEREOSEARCH FS

C25 H26 N2 O9 MF

SR CA

CA, CAPLUS, TOXCENTER, USPATFULL LC STN Files:

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1957 TO DATE)

4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:333118

REFERENCE 3: 137:247552

REFERENCE 4: 137:244598

L7 ANSWER 45 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN459809-56-4 REGISTRY

2-Naphthacenecarboxamide, 9-(aminomethyl)-7-butyl-4-(dimethylamino)-CN 1, 4, 4a, 5, 5a, 6, 11, 12a-octahydro-3, 10, 12, 12a-tetrahydroxy-1, 11-dioxo-, (4S, 4aS, 5aR, 12aS) - (9CI) (CA INDEX NAME)

FS STEREOSEARCH

C26 H33 N3 O7 MF

SR CA

CA, CAPLUS, TOXCENTER, USPATFULL LCSTN Files:

3 REFERENCES IN FILE CA (1957 TO DATE)

3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:247552

REFERENCE 3: 137:244598

L7 ANSWER 50 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 459809-46-2 REGISTRY

CN 3-Pyridinecarboxamide, N-[[(5aR,6aS,7S,10aS)-9-(aminocarbonyl)-7-(dimethylamino)-4-ethyl-5,5a,6,6a,7,10,10a,12-octahydro-1,8,10a,11-tetrahydroxy-10,12-dioxo-2-naphthacenyl]methyl]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C30 H32 N4 O8

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1957 TO DATE)

4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:333118

REFERENCE 3: 137:247552

REFERENCE 4: 137:244598

L7 ANSWER 55 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN * 389624-83-3 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-(2-pyridinylacetyl)-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H27 N3 O8

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1957 TO DATE)

4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:333118

REFERENCE 3: 137:244598

REFERENCE 4: 136:102232

L7 ANSWER 60 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 389624-73-1 REGISTRY

CN 2-Naphthacenecarboxamide, 7-(2-cyclohexylethyl)-4-(dimethylamino)1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-,
(4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H36 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

4 REFERENCES IN FILE CA (1957 TO DATE)

4 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:333118

REFERENCE 3: 137:244598

REFERENCE 4: 136:102232

L7 ANSWER 65 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 389624-63-9 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-7-[2-(2-pyridinyl)ethyl]-, (4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H29 N3 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

2 REFERENCES IN FILE CA (1957 TO DATE)

2 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 136:102232

L7 ANSWER 70 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 389624-39-9 REGISTRY

CN 2-Naphthacenecarboxamide, 4-(dimethylamino)-7-(3-ethylpentyl)1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-,
(4S,4aS,5aR,12aS)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C28 H36 N2 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1957 TO DATE)

5 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:333118

REFERENCE 3: 137:244598

REFERENCE 4: 137:244597

REFERENCE 5: 136:102232

L7 ANSWER 75 OF 75 REGISTRY COPYRIGHT 2003 ACS

RN 389624-01-5 REGISTRY

CN 2-Naphthacenecarboxamide, 7-[2-(4-aminophenyl)ethyl]-4-(dimethylamino)-1,4,4a,5,5a,6,11,12a-octahydro-3,10,12,12a-tetrahydroxy-1,11-dioxo-,(4S,4aS,5aR,12aS)-(9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H31 N3 O7

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

3 REFERENCES IN FILE CA (1957 TO DATE)
3 REFERENCES IN FILE CAPLUS (1957 TO DATE)

REFERENCE 1: 138:117673

REFERENCE 2: 137:333118

REFERENCE 3: 136:102232

=> d his

L8

(FILE 'HOME' ENTERED AT 12:12:12 ON 29 APR 2003) SET COST OFF

FILE 'REGISTRY' ENTERED AT 12:12:19 ON 29 APR 2003

L1 STR

L2 8 S L1

L3 166 S L1 FUL

SAV TEMP L3 GERSTL895/A

L4 STR L1

L5 5 S L4 SAM SUB=L3

L6 91 S L4 FUL SUB=L3

SAV L6 GERSTL895A/A TEMP

L7 75 S L3 NOT L6

FILE 'HCAPLUS' ENTERED AT 12:15:00 ON 29 APR 2003

9 S L6

L9 6 S L7

L10 6 S L8 AND L9

L11 9 S L8-L10

L12 9 S L11 AND (NELSON ? OR FRECHETTE ? OR VISKI ? OR ISMAIL ? OR BO

FILE 'HCAPLUS' ENTERED AT 12:17:19 ON 29 APR 2003

FILE 'USPATFULL, USPAT2' ENTERED AT 12:17:23 ON 29 APR 2003

L13 3 S L6

L14 2 S L7

L15 3 S L13, L14

FILE 'HCAPLUS, USPATFULL' ENTERED AT 12:17:39 ON 29 APR 2003 12 DUP REM L12 L15 (0 DUPLICATES REMOVED) L16

FILE 'REGISTRY' ENTERED AT 12:18:00 ON 29 APR 2003

FILE 'USPATFULL, USPAT2' ENTERED AT 12:18:15 ON 29 APR 2003

FILE 'HCAPLUS' ENTERED AT 12:18:28 ON 29 APR 2003

FILE 'REGISTRY' ENTERED AT 12:18:54 ON 29 APR 2003